

# Computing Sciences at Berkeley Lab

**Katherine Yelick NERSC Director** 





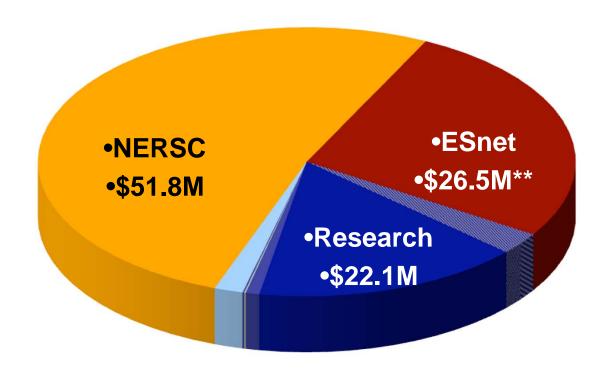
# Computing Sciences Mission

- Deliver world class facilities, NERSC and ESnet, supporting the DOE Office of Science computational mission
- Conduct world class research in applied mathematics and computer science in support of DOE science mission
- Build and maintain an outstanding computational science and engineering (CSE) research effort in close collaboration with the UC campuses



# Computing Science Programs

\$100.3M\* Annual Budget in FY09



- •\*\$3M deducted from FY09 NERSC budget for funds received in FY08
- •\*\* ESnet includes 3.2M for services provided to other sites through IWOs











#### COMPUTING SCIENCES DIRECTORATE

HORST SIMON
Associate Laboratory Director for Computing Sciences

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NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING (NERSC) DIVISION

KATHY YELICK Division Director

HOWARD WALTER
Division Deputy

SYSTEMS DEPARTMENT

Jeff Broughton
Department Head

SERVICES DEPARTMENT

FRANCESCA VERDIER
Department Head

**COMPUTATIONAL RESEARCH DIVISION** 

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Division Deputy

ADVANCED COMPUTING FOR SCIENCE

DEBORAH AGARWAL
Department Head

BIOLOGICAL DATA
MANAGEMENT CENTER

VICTOR MARKOWITZ

Department Head

HIGH PERFORMANCE COMPUTING RESEARCH DEPARTMENT

JUAN MEZA
Department Head

Michael Banda

**CS DEPUTY** 

ENERGY SCIENCES NETWORK
(ESnet)

STEVEN COTTER
Department Head

JOSEPH BURRESCIA General Manager **BUSINESS MANAGEMENT** 

COMMUNICATIONS

**FACILITIES AND EH&S** 

**HUMAN RESOURCES** 

**Kathy Yelick** 









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**HUMAN RESOURCES** 

FUTURE TECHNOLOGIES GROUP

Erich Strohmaier Group Lead





# Overview of the Berkeley UPC Project



# **UPC Project Goals**

#### 2001-2004: A Portable UPC Compiler

- UPC was (incorrectly) viewed as a language that required shared memory hardware or only ran on Cray machines
- The Berkeley UPC compiler showed it could run on clusters with a lightweight runtime and that source-to-source translation was reasonable

### 2005-2008: UPC is a High Performance Language

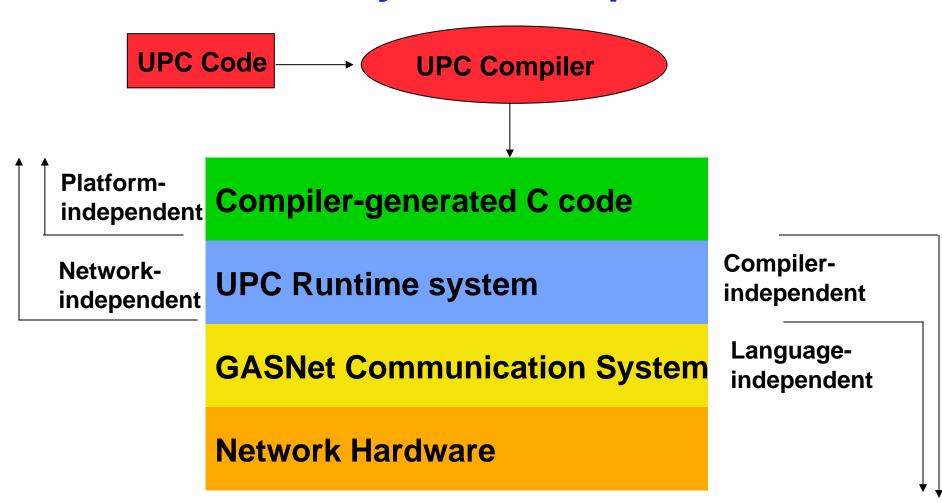
- Conventional wisdom: UPC is more productive than MPI but we should expect it to be slower (maybe by 2x)
- Even on clusters without global address space support, UPC can outperform MPI on microbenchmarks and apps

### 2008-2010: UPC for multicore & hybrid multicore / clusters

- Are either MPI / core or OpenMP within a node "good enough"?
- UPC should be better: lower memory footprint, better locality contol



### Berkeley UPC Compiler



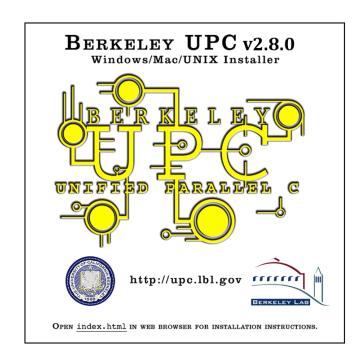




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# **Berkeley UPC Compiler Highlights**

- Portable, high-performance open-source UPC compiler
  - Fully UPC spec compliant
  - Includes UPC collectives and UPC-I/O
- Many extensions for performance and programmability
  - Non-blocking and non-contiguous memcpy functions
  - Semaphores and signaling put
  - Fine granularity timers
  - Value-based collectives
  - Atomic memory operations
  - Hierarchical layout query
  - Call to/from MPI (C++, F, etc.)
- Entirely free & open source
  - Available from <a href="http://upc.lbl.gov">http://upc.lbl.gov</a>
  - Also in CDs at SC each year



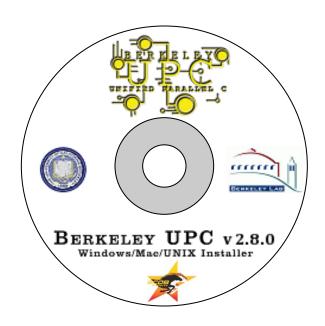




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### New in November 2008 Release

- Native support for IBM BlueGene/P (dcmf conduit)
- Cray Portals network upgrade to cache local memory registration
- Many small improvements to IBM LAPI support
- Improvements in Myrinet GM support
- InfiniBand support for InfiniPath adapters
- Experimental support for ARM processors
- MIPSEL/Linux (SiCortex) support (alas)
- Fine-grained programs optimizations split-phase, access coalescing
- Beta release of "vectorization"
- Pathscale Compiler support
- Many bug fixes





# Multicore (and Accelerator) Plans

- Performance is often non-obvious
  - E.g., MPI faster than threads on an SMPs
- Multiple runtime approaches
  - SMP runtime system based on Pthreads (old)
    - Some work to pin threads and get memory affinity for NUMA
    - Some overhead for thread-local (globally scoped) data
  - Run a GASNet conduit with processes
    - High overhead for communication, but good data partitioning
  - Processes with some form of OS-supported shared memory
    - Prototype done by Jason Duell, but only for a single node
    - More from Filip today
- Partitioned memory space (GPUs, Cell, etc.)
  - Some work on this by Filip for Cell
  - More ideas from Yili and rest of the group





### **Collective Communication**

### Important for many scientific applications

- Productivity and performance enhancer
- Teams are critical: more on this later by Yili

#### Collectives for clusters

- Work with IBM, data centric
- New work: completely re-designed and re-built collectives
- Some improvements in Nov 08 release, more coming

#### Collectives for Multicore

Surprisingly important, even for barriers

### Autotuned collectives (Yili and Rajesh)

Taking the pain out of tuning





### **GASNet**

- Focus on BG/P conduit (Rajesh)
  - Scaling work on Intrepid machine at Argonne (ALCF)
- Cray Portals conduit (Paul)
  - Several bug fixes and performance improvements
  - Ongoing benchmarking work on Franklin machine at NERSC and others

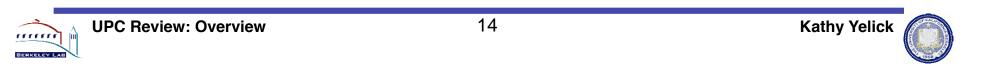
#### Infiniband

- Ongoing bug fixed and performance improvements
- Work specifically on scaling for Ranger machine at TACC



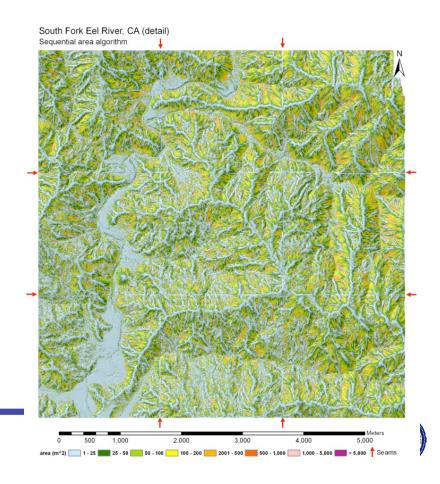
# **UPC Applications from LBNL**

- UPC applications stress global address space:
  - irregular remote memory accesses
  - need for low overhead communication
- Delaunay mesh generation
- Adaptive Mesh Refinement
- Sparse Cholesky factorization
- Biology application
- Dense LU factorization with event-driven execution
- Latest one: Landscape evolution (NSF PetaApps Climate project)



# Landscape Evolution

- How to evolve landscapes over time?
  - · Erosion, rainfall, river incision
- Area distribution
  - Want to parallelize this
- Input series of tiles
  - Vast input range
  - Serial seams





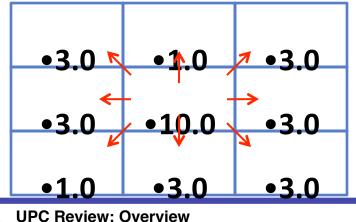
# Area Distribution Algorithm

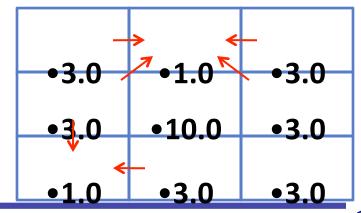
### Analogous to precipitation distribution

- Each cell seeded with an initial area distribution
- Area "distributed" proportionally to downhill neighbors based on elevation

### Originally a recursive, serial algorithm

Changed to a scatter operation for parallel implementation

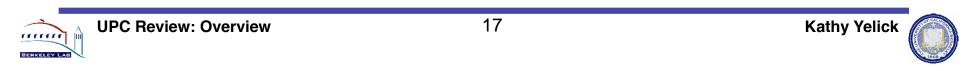






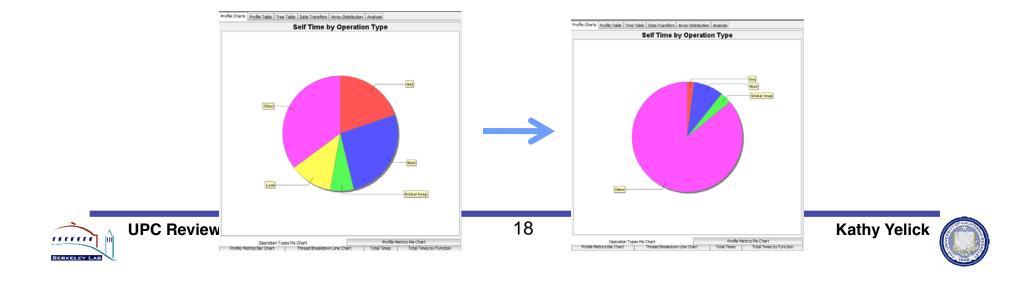
# **UPC** Implementation

- Input elevation tiles stored in global shared array
  - Threads split input tiles with horizontal stripes
- Information shared after collecting all uphill data
  - Reduces communication across threads
  - Queues used to push/pop information to/from remote threads
- Threads alternate work between local/remote queues to improve throughput
- Computation ceases once all cells have pushed data



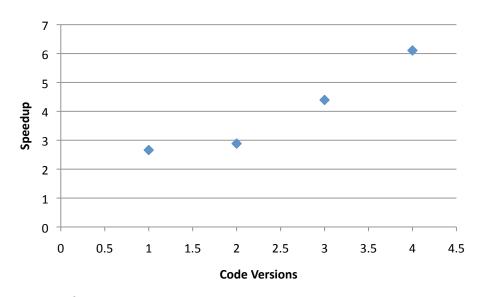
### **Implementations**

- Original implementation was very inefficient
  - Remote variables, upc\_locks, non-local queues
- PPW helpful in locating areas of inefficiency
  - Indicated areas in source with unexpected communication
  - UPC functions comprised > 60% of runtime



# **Optimizations**

- V 1 Optimized parallel base-code
- V 2 Remote queues local to data owner
- V 3 Replaced queues with dynamic arrays for local computation
- V 4 Replaced UPC locks with semaphores



Tests performed with eight 2km x 2km tiles and eight threads





# **Analysis**

- Speedup capped by topography
  - In worst case, performance could be less than serial code
  - In best case, with minimal computation, can achieve a speedup of 7.1 for prior test case
- Eliminating UPC locks gave best results in terms of scalability
- PPW helpful for pinpointing areas for improvement
- Running algorithm in parallel is only way to achieve the true results



9:00 a.m.	Overview of Computing Sciences and	Kathy Yelick
	Berkeley UPC Project	
9:30 a.m.	Berkeley Compiler Update	Costin lancu
10:00 a.m.	Intrepid Compiler Update	Gary Funck
10:30 a.m.	Break	
10:45 a.m.	Team Collectives and BG/P Results	Yili and Rajesh
11:30	GASNet on Cray Portals	Paul Hargrove
12:00 p.m.	Working Lunch	
	Process-Based SMP Runtime	Filip Blagojevic
1:00 p.m.	Autotuned Multicore Collectives	Rajesh Nishtala
1:30 p.m.	Resource Management for Multicore	Costin lancu
2:15 p.m	Compiling Shared Memory programs for GPUs	Seung-Jai Min
2:40 p.m.	UPC Ideas for GPUs / Accelerators	Yili Zheng
3:15 p.m.	Break	
3:30 p.m.	Irregular Communication Optimizations in PGAS	Jimmy Su
4:00 p.m.	Irregular Memory Optimizations on Multicore	Kamesh Madduri
4:30 p.m.	Future Plans	Kathy Yelick



